Energy Levels of Quasiperiodic Hamiltonians, Spectral Unfolding, and Random Matrix Theory

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February 1, 2008

Abstract

We consider a tight-binding Hamiltonian defined on the quasiperiodic Ammann-Beenker tiling. Although the density of states (DOS) is rather spiky, the integrated DOS (IDOS) is quite smooth and can be used to perform spectral unfolding. The effect of unfolding on the integrated level-spacing distribution is investigated for various parts of the spectrum which show different behaviour of the DOS. For energy intervals with approximately constant DOS, we find good agreement with the distribution of the Gaussian orthogonal random matrix ensemble (GOE) even without unfolding. For energy ranges with fluctuating DOS, we observe deviations from the GOE result. After unfolding, we always recover the GOE distribution.

In two recent papers [1, 2], we investigated the energy-level statistics of two-dimensional quasiperiodic Hamiltonians, concentrating on the case of the eight-fold Ammann-Beenker tiling [3] shown in Fig. 1. The Hamiltonian contains solely constant hopping elements along the edges of the tiles in Fig. 1. Numerical results suggest that typical eigenstates of the model are multifractal [4]. In [1, 2], we numerically calculated the level-spacing distribution $P(s)$ and the Δ_3 and Σ_2 statistics [5], and found perfect agreement with the results for the GOE. One ingredient of the calculation was the so-called unfolding procedure, explained below, which corrects for the fluctuations in the DOS of the model Hamiltonian. It is well known that, for

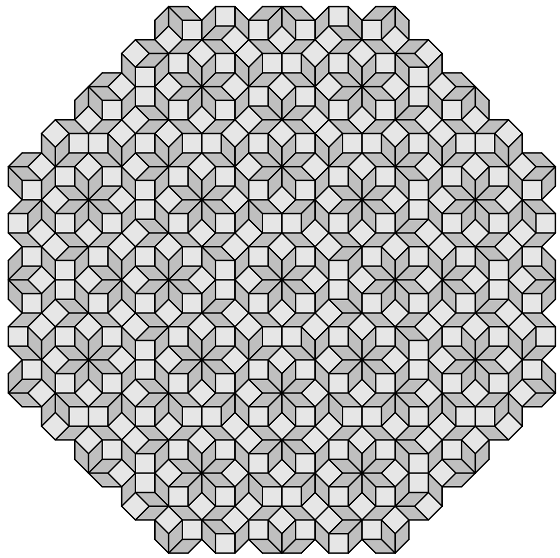

Figure 1: Octagonal cluster of the Ammann-Beenker tiling with 833 vertices and an exact D_8 symmetry around the central vertex.

a spectrum with non-constant DOS, it is necessary to unfold the spectrum in order to extract universal level statistics which can then be compared to the results of random matrix theory [5].

In the present paper, we trace the question how crucial the unfolding procedure affects the universal results, restricting ourselves to the integrated level-spacing distribution (ILSD) $I(s) = \int_s^\infty P(s')\,ds'$. In previous studies of the model [6, 7, 8], spectral unfolding had not been used, the main reason being that the DOS is rather spiky as shown in Fig. 2. In [9], it was claimed that the level-spacing distribution (LSD) depends crucially on the unfolding, yielding results ranging from log-normal to GOE behaviour. In fact, if one considers the IDOS which is also shown in Fig. 2, one finds that it is rather smooth, apart from a couple of small gaps and a jump at energy $E = 0$ caused by the existence of 13077 degenerate states in the band center [1]. These states can be neglected for the level-spacing distribution since they only contribute to $P(0)$. Therefore, we use the IDOS to unfold the energy spectra.

The purpose of the spectral unfolding is to transfer a spectrum with a non-constant DOS to the another with a unit DOS or a linear IDOS.

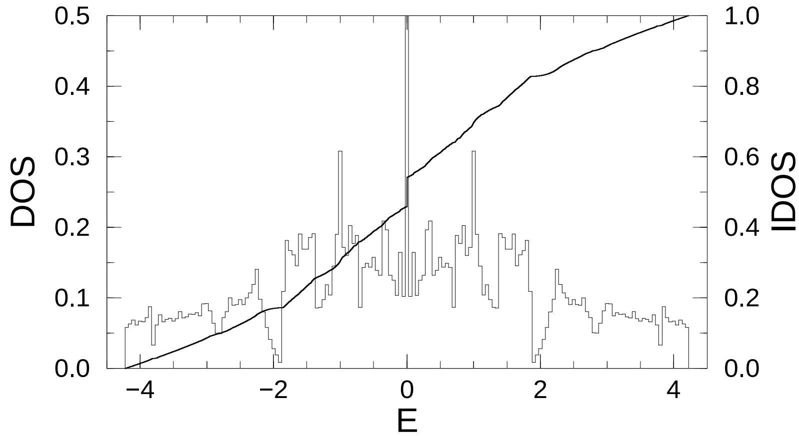

Figure 2: DOS and IDOS for a D_8-symmetric patch with 157369 vertices.

In order to achieve this, one defines the unfolded levels as $e_i = N_{\rm av}(E_i)$, where E_i is the i-th energy level, $N_{\rm av}(E_i)$ the smoothened IDOS [5]. Level spacings are thus given by $s_i = e_{i+1} - e_i$. An effective way to calculate the $N_{\rm av}(E_i)$ is to fit the IDOS to cubic splines by choosing a sequence of energy levels $(E_1, E_{m+1}, E_{2m+1}, \ldots)$ from the energy spectrum $(E_1, E_2, \ldots, E_n)$. A meaningful statistics should be independent of the unfolding parameter m. Evidently, the value of m, which does not change the statistics, depends on the total number of levels n and the structure of the DOS. The typical value for the Anderson Hamiltonian is around 100 [10, 11].

The eight-fold Ammann Beenker tiling shown in Fig. 1 has the full D_8 symmetry of the regular octagon, hence the Hamiltonian matrix splits into ten blocks according to the irreducible representations of the dihedral group D_8, resulting in seven different independent subspectra as there are three pairs of identical spectra. In order to obtain the underlying universal LSD, one should consider the irreducible subspectra seperately [1, 5]. In the following, we demonstrate our results by concentrating on one of the largest subspectra of the Ammann Beenker D_8-symmetric tiling of 157369 vertices. We note that the derived conclusions hold for all the subspectra. Fig. 3 shows level spacing distributions for energy levels in various parts of the spectrum without and with unfolding. It is easy to see from Fig. 3(a) that energy levels with an approximately constant DOS (for instance, $3.2 \leq E \leq 3.3$) exhibit GOE behaviour even without unfolding. However, for energy ranges

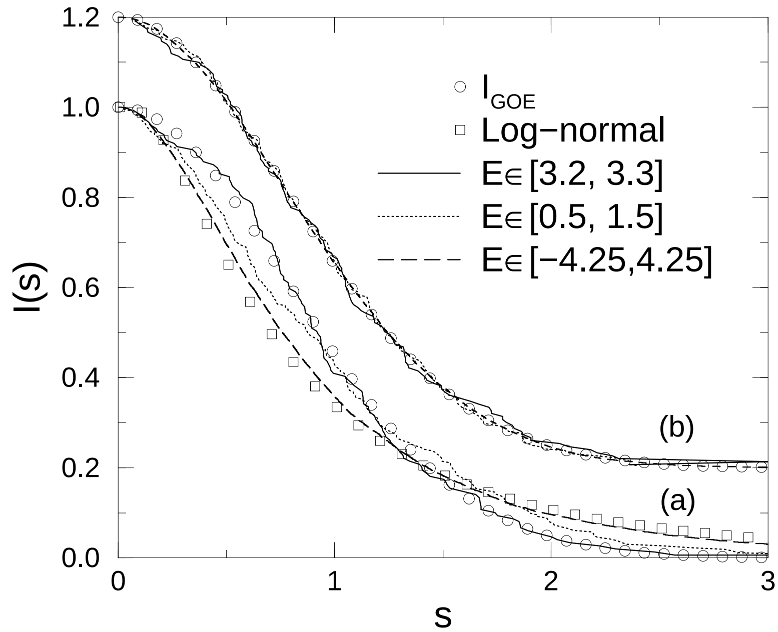

Figure 3: ILSD $I(s)$ obtained (a) without unfolding and (b) with unfolding for various parts of the spectrum of one sector of the D_8-symmetric patch: whole spectrum (dashed line), $0.5 \leq E \leq 1.5$ (dotted line), and $3.2 \leq E \leq 3.3$ (solid line). Circles and boxes denote $I_{\mathrm{GOE}}(s)$ and the log-normal distribution, respectively. $I(s)$ in (b) has been shifted by 0.2 for clarity.

with fluctuating DOS, $I(s)$ apparently deviates from the $I_{\mathrm{GOE}}(s)$ if we do not perform the unfolding. For instance, $I(s)$ for the non-unfolded whole spectrum is close to the log-normal distribution although the log-normal distribution is not the generic level statistics of the quasiperiodic Hamiltonian. Analyzing the non-unfolded spectrum in the range with the largest fluctuations, $0.5 \leq E \leq 1.5$, one can clearly see that $I(s)$ is neither log-normal nor GOE. From Fig. 3(b), we can see that, after the unfolding, $I(s)$ for different energy intervals show a very good agreement with the GOE result.

In our calculation, we find that there exists a sequence of m ranging from 4 to 30, which gives the same statistics described by $I_{\mathrm{GOE}}(s)$, within our numerical precision. In Fig. 4, we illustrate $I(s)$ obtained with $m = 5, 10$, 20, and 100. One can see that there is only a small deviation from the $I_{\mathrm{GOE}}(s)$ even for large m up to 100. We emphasize that even for such a large

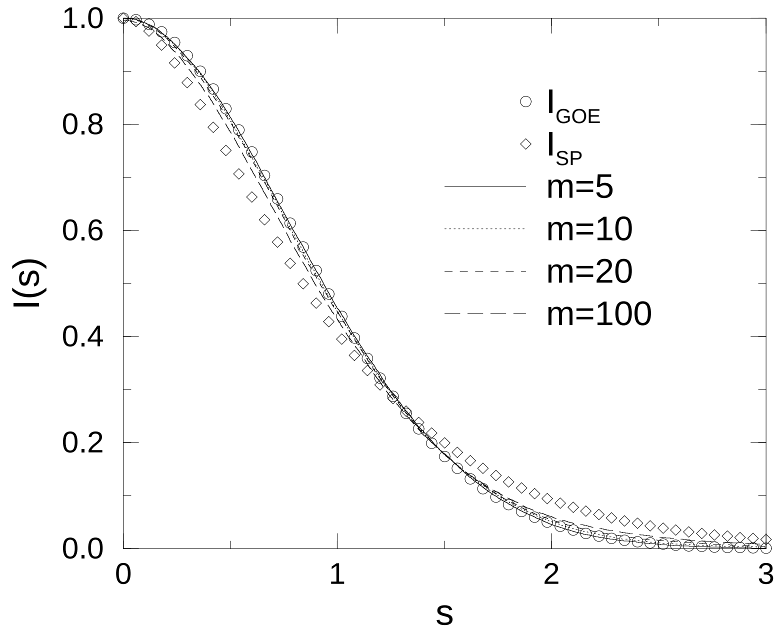

Figure 4: ILSD $I(s)$ obtained for one sector of the D_8-symmetric patch with different parameters m in the unfolding procedure. The result is compared to $I_{\mathrm{GOE}}(s)$ (circles) and the intermediate ("semi-Poisson") statistics $I_{\mathrm{SP}}(s)$ (diamonds).

m, $I(s)$ is still far from the so-called "semi-Poisson" intermediate statistics $I_{\mathrm{SP}}(s) = (2s+1)e^{-2s}$ [12], which is supposed to be valid to describe the level statistics at the metal-insulator transition with multifractal eigenstates in the three-dimensional Anderson model of localization.

In summary, we have shown that although the DOS of the quasiperiodic tight-binding Hamiltonian defined on the Ammann-Beenker tiling exhibits very spiky structures, the IDOS is in fact rather smooth and can be used to perform spectral unfolding. We demonstrated that the level spacing distribution is independent of the unfolding parameter and is well described by the GOE distribution. We also studied the level statistics for energy spectra without unfolding and found that, for energy intervals with approximately constant DOS, $I(s)$ agrees with the GOE distribution; for energy ranges with fluctuating DOS, $I(s)$ varies with different energy intervals and the log-normal distribution found in a previous calculation [7] is not generic.

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